

NaNbO₃ Structure:

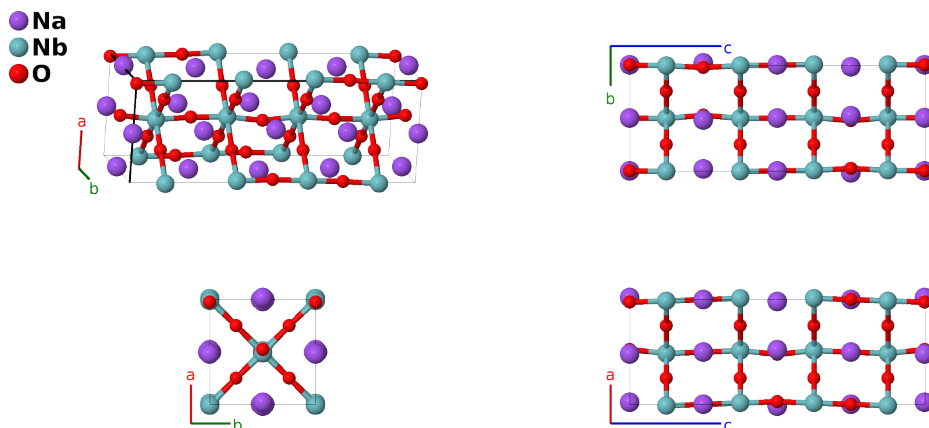
ABC3_oP40_17_abcd_2e_abcd4e-001

This structure originally had the label `ABC3_oP40_17_abcd_2e_abcd4e`. Calls to that address will be redirected here.

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<https://afLOW.org/p/D6BJ>

https://afLOW.org/p/ABC3_oP40_17_abcd_2e_abcd4e-001



Prototype	NaNbO ₃
AFLOW prototype label	ABC3_oP40_17_abcd_2e_abcd4e-001
ICSD	76432
Pearson symbol	oP40
Space group number	17
Space group symbol	$P222_1$
AFLOW prototype command	<code>afLOW --proto=ABC3_oP40_17_abcd_2e_abcd4e-001</code> <code>--params=$a, b/a, c/a, x_1, x_2, x_3, x_4, y_5, y_6, y_7, y_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$</code>

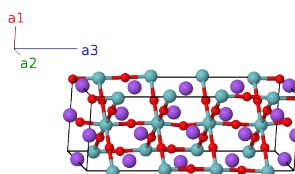
- (Downs, 2003) identifies this as a “possible polymorph of lueshite.”
- If the aflow parameters are set to `--params= $a, 1, \sqrt{8}, 1/2, 0, 0, 1/2, 1/2, 0, 0, 1/2, 0, 0, 3/8, 1/2, 1/2, 3/8, 1/4, 1/4, 3/8, 3/4, 1/4, 3/8, 1/4, 3/4, 3/8, 3/4, 3/4, 3/8$` then the structure is equivalent to cubic perovskite $E2_1$.

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{x}$$

$$\mathbf{a}_2 = b \hat{y}$$

$$\mathbf{a}_3 = c \hat{z}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1$	$=$	$ax_1 \hat{\mathbf{x}}$	(2a)	Na I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Na I
\mathbf{B}_3	$= x_2 \mathbf{a}_1$	$=$	$ax_2 \hat{\mathbf{x}}$	(2a)	O I
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(2b)	Na II
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Na II
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(2b)	O II
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	O II
\mathbf{B}_9	$= y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Na III
\mathbf{B}_{10}	$= -y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Na III
\mathbf{B}_{11}	$= y_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	O III
\mathbf{B}_{12}	$= -y_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	O III
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	Na IV
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	Na IV
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	O IV
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	O IV
\mathbf{B}_{17}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4e)	Nb I
\mathbf{B}_{18}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Nb I
\mathbf{B}_{19}	$= -x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Nb I
\mathbf{B}_{20}	$= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4e)	Nb I
\mathbf{B}_{21}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4e)	Nb II
\mathbf{B}_{22}	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Nb II
\mathbf{B}_{23}	$= -x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Nb II
\mathbf{B}_{24}	$= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4e)	Nb II
\mathbf{B}_{25}	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4e)	O V
\mathbf{B}_{26}	$= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O V
\mathbf{B}_{27}	$= -x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O V
\mathbf{B}_{28}	$= x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4e)	O V
\mathbf{B}_{29}	$= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(4e)	O VI
\mathbf{B}_{30}	$= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VI
\mathbf{B}_{31}	$= -x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VI
\mathbf{B}_{32}	$= x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(4e)	O VI
\mathbf{B}_{33}	$= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(4e)	O VII
\mathbf{B}_{34}	$= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VII
\mathbf{B}_{35}	$= -x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VII
\mathbf{B}_{36}	$= x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}}$	(4e)	O VII
\mathbf{B}_{37}	$= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	(4e)	O VIII
\mathbf{B}_{38}	$= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VIII

$$\mathbf{B}_{39} = -x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3 = -ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4e) \quad \text{O VIII}$$

$$\mathbf{B}_{40} = x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 = ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} \quad (4e) \quad \text{O VIII}$$

References

- [1] P. Vousden, *The Structure of Ferroelectric Sodium Niobate at Room Temperature*, Acta Cryst. **4**, 545–551 (1951), doi:10.1107/S0365110X51001768.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).